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LECTURES ON MATHEMATICAL COMBUSTION

Lecture 9: Spherical Diffusion Flames

Technical Report No. 154

J.D. Buckmaster & G.S.S. Ludford

January 1983

Theoretical and Applied Mechanics

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Thurston Hall
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Contents

Lecture 9

SPHERICAL DIFFUSION FLAMES

Law has shown that the analysis of spherical diffusion flames is quite similar to that of counterflow diffusion flames, so that some explanation is needed for devoting a separate lecture to them. There are two good reasons. First, the constant-density approximation has been used throughout these lectures in discussing all but plane flames, so there is room for a problem which does not neglect variations in density. (Plane diffusion flames have to be chambered, i.e. the reactants must be supplied at finite locations, which leads to distracting complications.) Secondly, the spherical diffusion flame can lead to quite different (and unusual) responses. These arise in the technologically important application to the quasi-steady phase of fuel-drop burning, when a more realistic boundary condition than the conventional one is used.

1. Basic Equations

The fuel is supposed to be supplied as a liquid at the surface of a sphere of radius a (figure 1), where the heat from a concentric flame sheet evaporates it. In turn, the flame sheet is sustained by the reaction of the gaseous fuel and oxidant in the ambient atmosphere. If the representative mass flux M_r is taken to be $\lambda/c_p a$, then a is the length unit. The density at infinity will be used for ρ_r.

We seek a spherically symmetric, steady solution of the full equations (2.18-20) under the assumption of unit Lewis numbers for the reactants. The equation of continuity integrates immediately to

$$r^2 \rho v = M \text{ (const.)}, \tag{1}$$

where M is loosely called the burning rate. (The liquid fuel evaporates

at the rate $4\pi M$, but the gaseous fuel only burns at that rate if there is
no outflow of fuel at infinity.) Although the radial velocity v is not
determined by this result, the thermal-chemical equations (2.20) are
uncoupled from the fluid-mechanical equations (2.18b,19) because, under
steady conditions, they only involve the mass flux ρv, which is determined
(as M/r^2). Once T is found, the density follows from

$$\rho T = T_\infty, \tag{2}$$

and then v is known; the momentum equation (2.19) serves only to determine
the pressure field.

We have to deal once more with equations (8.2), where now, however,

$$L \equiv \frac{M}{r^2} \frac{d}{dr} - \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr}. \tag{3}$$

The boundary conditions are

$$T = T_s, \ dT/dr = ML, \ X-M^{-1}dX/dr = 0, \ Y-M^{-1}dY/dr = 1 \text{ at } r = 1, \tag{4}$$

$$T \to T_\infty, \ X \to X_\infty, \ Y \to 0 \text{ as } r \to \infty, \tag{5}$$

where T_s, L, T_∞, X_∞ are given. Prescription of the surface temperature
T_s will later be replaced by the requirement of liquid-vapor equilibrium;
the latent heat of evaporation L is positive; the conditions (4c,d) ensure
that the sphere is a source of fuel, but neither a source nor sink of
oxidant (or anything else); the prescribed oxidant fraction at infinity
must of course satisfy $0 < X_\infty \leq 1$; and the condition (5c) ensures that
all the fuel has originated at the supply.

The sixth-order system of differential equations is therefore subject
to seven boundary conditions, as a consequence of which M is determined
as a function of $\mathcal{D}$ (depending also on T_s, L, T_∞, and X_∞). The maximum
temperature could be used to characterize the solution, as for the counterflow

diffusion flame, but we shall use M instead. The burning rate is of greater interest in applications, and it arises naturally in the analysis.

The Shvab-Zeldovich relations are

$$T+2X = (T_s-L)(1-e^{-M/r})+(T_\infty+2X_\infty)e^{-M/r} \equiv Z_-(M), \qquad (6)$$

$$T+2Y = T_\infty+(T_a-T_\infty)(1-e^{-M/r}) \equiv Z_+(M), \qquad (7)$$

where

$$T_a = T_s-L+2$$

is called the adiabatic flame temperature. For $T_\infty = T_a$, no heat is conducted to or from the ambient atmosphere when (as is usually the case) $Y = o(r^{-1})$ as $r \to \infty$; this conclusion follows from the relation (7), which gives

$$\lim_{r\to\infty}(4\pi r^2 dT/dr) = \lim_{r\to\infty} [4\pi r^2(T_a-T_\infty)(-Me^{-M/r}/r^2)] = 4\pi M(T_\infty-T_a). \qquad (8)$$

We further see that

$$T_a > T_\infty \qquad (9)$$

will ensure the conduction of heat to the environment, the aim of combustion in practice.

The problem now reduces to one for T alone, namely

$$L(T) = \mathcal{D}XYe^{-\theta/T}, \quad T = T_s, \quad dT/dr = ML \quad \text{at } r = 1, \quad T \to T_\infty \text{ as } r \to r_\infty, (10)$$

where X and Y are to be suppressed in favor of T by means of the Shvab-Zeldovich relations (6), (7). We shall first derive the frozen $(\mathcal{D}e^{-\theta/T} \to 0)$ and equilibrium $(\mathcal{D}e^{-\theta/T} \to \infty)$ limits of the solution.

For frozen combustion, start by setting

$$\epsilon^2 = \tfrac{1}{2}\mathcal{D}X_\infty e^{-\theta/T_\infty} \tag{11}$$

equal to zero. We find

$$T = T_s - L + L e^{M_w(1-1/r)} \quad \text{with} \quad M_w \equiv \ln[1+(T_\infty-T_s)/L] \tag{12}$$

where, since Y must be positive,

$$M_w > 0, \text{ i.e. } T_\infty > T_s. \tag{13}$$

This is the pure evaporation solution with no combustion; the environment must be hotter than the surface in order to supply the heat necessary to vaporize the liquid. (There is no condensation solution.) The result is not uniformly valid, since for $r = O(\epsilon^{-1})$ the reaction term is comparable to the convection term in the equation (10a). The variable

$$R = \epsilon r \tag{14}$$

leads to the expansion

$$T = T_\infty - \epsilon M_w[T_\infty - T_s + L - 2(1-e^{-R})]/R + \ldots, \tag{15}$$

The frozen limit is not an extinguished state, but rather one in which all the reaction takes place at essentially constant temperature far from the supply.

Turning now to the (Burke-Schumann) equilibrium limit, we use the Shvab-Zeldovich relations (6), (7) to obtain

$$T = \begin{cases} Z_-(M_e) \\ Z_+(M_e) \end{cases}, \quad X = \begin{cases} 0 \\ (1+X_\infty)e^{-M_e/r} - 1 \end{cases}, \quad Y = \begin{cases} 1-(1+X_\infty)e^{-M_e/r} \\ 0 \end{cases} \quad \text{for } r \lessgtr r_*, \tag{16}$$

where the boundary condition (10b) fixes

$$M_e \equiv \ln[1+(T_\infty-T_s+2X_\infty)/L] \qquad (17)$$

and the continuity of X and Y across the flame sheet requires

$$r_* = M_e/\ln(1+X_\infty). \qquad (18)$$

The flame temperature, i.e. the common value to which T tends as $r \to r_* \pm 0$, is

$$T_* = T_\infty + \gamma X_\infty \text{ with } \gamma = (T_a-T_\infty)/(1+X_\infty). \qquad (19)$$

For consistency, the value (18) of r_* must be greater than 1, i.e.

$$T_\infty-T_s > (L-2)/X_\infty. \qquad (20)$$

While this condition is automatically met when the inequalities (9), (13b) are satisfied (as they are in the practically important case to which we shall limit our later discussion) it is of interest to note that there is a second limit, found by Buckmaster, when the condition is violated. The flame sheet lies at the surface itself, instead of some distance away, so that there is no oxidant-free region.

The flame-sheet structure in the Burke-Schumann limit is the same irrespective of whether the counterflow or spherical diffusion flame is being considered (cf. end of section 8.1). The continuity conditions

$$\delta(T) = \delta(X) = \delta(Y) = 0 \qquad (21)$$

are required for a structure to exist, but the gradients of T, X, and Y are different on the two sides of the flame sheet because the latter is a source of heat and a sink of both reactants. The Shvab-Zeldovich relations show, however, that

$$\delta(dT/dr+2dX/dr) = \delta(dT/dr+2dY/dr) = 0. \qquad (22)$$

2. Nearly Adiabatic Burning

We turn now to the full response curve $M(\mathcal{D})$ in the limit $\theta \to \infty$, noting once again that the burning rate is a more convenient and significant parameter than the maximum temperature to characterize the solution. Here the response is S-shaped if T_s, L, T_∞ satisfy the inequalities (9) and (13b), i.e. when the heat flux (8) is to the environment, as required in practice, and the surface temperature is less than that of the ambient atmosphere. The transition from an S-shaped response to a monotonic one occurs, for large activation energy, when the temperature gradient (i.e. the heat flux) beyond the flame is small, so that it may be described by setting

$$T_a - T_\infty = k/\theta \quad \text{with} \quad k = \text{const.;} \tag{23}$$

here T_∞ and L are supposed fixed as T_s varies. The inequality (13b) which ensures a weak-burning branch for the response, requires

$$L < 2. \tag{24}$$

Note that the requirement (20) for the Burke-Schumann limit is automatically satisfied, ensuring a strong-burning branch of that form.

Equilibrium will be assumed behind the flame sheet even though the temperature does not rise above T_* ($= T_\infty$, to leading order) there by an $O(1)$ amount. The combustion is frozen between the surface and the flame sheet, because of the requirement (13b). The Shvab-Zeldovich relation (7) therefore gives us

$$T = T_\infty + (k/\theta)(1 - e^{-M/r}) \quad \text{for} \quad r > r_*, \tag{25}$$

in view of the assumption (23); and the boundary conditons (10b,c) lead to

$$T = T_s - L + Le^{M(1-1/r)} \text{ for } r < r_*. \tag{26}$$

These formulas are correct to any order in θ^{-1}, provided that M is determined to the same order; we shall only need a leading-order determination of M, and that will be understood in what follows. Leading-order continuity of T now shows that

$$r_* = M/[M+\ln(L/2)], \tag{27}$$

a result that exhibits the need for the inequality (24). To analyz he reaction zone we shall also need the leading-order result

$$X_* = (1+X_\infty)e^{-M/r*}-1, \tag{28}$$

coming from the Shvab-Zeldovich relation (6).

Determination of M comes from analysis of the reaction zone, for which the appropriate variable is

$$\xi = \theta(r-r_*). \tag{29}$$

Coefficients in the layer expansion

$$T = T_\infty - \theta^{-1}T_\infty^2\phi + \ldots \text{ with } \phi = (1/T)_1 \tag{30}$$

are considered to be functions of ξ. The Shvab-Zeldovich relation gives

$$Y = \tfrac{1}{2}\theta^{-1}T_\infty^2(\phi-\phi_*)+\ldots \text{ with } \phi_* = -k(1-e^{-M/r_*})/T_\infty^2, \tag{31}$$

so that the structure is governed by equation (8.24) with T_{f+} replaced by T_∞. As there, the structure equation provides an expression for the temperature gradient in the field (26) in front of the flame sheet, whence we find the equation

$$\frac{2M}{r_*^2} = \frac{T_\infty^2 \sqrt{\mathcal{D}X_*} \; e^{-\phi_*/2}}{\theta e^{\theta/T_\infty}} \qquad (32)$$

for M as a function of $\mathcal{D}$. This function can be defined parametrically, as for the counterflow diffusion flame at the end of section 8.2. Thus, M is given as a function of r_* by the formula (27), and then $\mathcal{D}$ is determined as a function of r_* by equation (32) with the substitutions (28) and (31b) for X_* and ϕ_*.

The corresponding response curve is shown in figure 2 for several values of k. The curve joins the frozen limit (12b) to the Burke-Schumann limit (17), monotonically if k is not too positive but otherwise via an S. Reponses in the shape of an S appear to be associated with a flux of heat from the flame sheet to an environment that is hotter than the supply surface, the normal state of affairs in practice. However, it has never been proved that the inequalities (9) and (13b) will ensure an S-response in the limit $\theta \to \infty$.

3. General Extinction and Ignition Analyses

The general extinction analysis under the conditions (9,13b) follows that for the counterflow diffusion flame in section 8.3. On the whole upper branch of the S-response, the burning rate lies within $O(\theta^{-1})$ of the value (17), so that we write

$$M = M_e + \theta^{-1} M_1 + \dots \qquad (33)$$

The combustion field on each side of the flame sheet is again frozen but identical to the equilibrium solution, here given by equations (16), so far as leading terms are concerned. However, we now need

$$T_1 = M_1 L(1-1/r) e^{M_e(1-1/r)} \qquad \text{for } r < r_* \qquad (34)$$

also, involving the perturbation M_1. It provides the stronger matching condition

$$\tilde{\phi} = -\tilde{\xi} - \tilde{M}_1 + \dots \text{ as } \xi \to -\infty \text{ with } \tilde{M}_1 = (1+\tilde{\gamma})M_1/T_*^2 \tag{35}$$

in the canonical problem (8.32,33), at which the analysis finally arrives with

$$\tilde{\gamma} = 1-\gamma, \quad \tilde{D}_e = r_*^4 \, T_*^8 \, D/4M_e^2\theta^3 e^{\theta/T_*}; \tag{36}$$

here r_*, T_*, and γ have the definitions (18) and (19).

Since the problem is well posed under the weaker condition, it follows that

$$\tilde{M}_1 = -\lim_{\xi \to -\infty} (\bar{\phi} + \tilde{\xi}) \tag{37}$$

can be calculated as a function of $\tilde{D}_e$, thereby determining the response. This response is shown in figure 3 for various values of γ; it has been found numerically, but not yet been proved, that the curve turns to form a C whenever γ is positive, consistent with the conjecture that the inequality (9) must hold for an S-response.

The general ignition analysis that was promised in section 8.6 will now be presented. The starting point is the analog of the assumption (33), namely

$$M = M_w + \theta^{-1}M_1 + \dots, \tag{38}$$

where M_w has the frozen value (12b). Correspondingly, the reaction all takes place far from the surface, the combustion field being frozen to all orders at any finite r. (The latter is ensured by the inequality (13b).)

Thus, the formulas

$$T_0 = T_s - L + Le^{M_w(1-1/r)}, \quad T_1 = M_1 L(1-1/r)e^{M_w(1-1/r)} \tag{39}$$

are obtained by satisfying conditions (10b,c) at the surface; but these do not satisfy the condition (10d) at infinity.

The appropriate variable at large distances is

$$R = r/\theta, \tag{40}$$

and then coefficients in the expansion (30) are to be considered functions of R. The equation for ϕ is

$$\frac{1}{R^2}\frac{d}{dR}\left(R^2 \frac{d\phi}{dR}\right) = \mathcal{D}_w\left[\phi + \frac{(T_a - T_\infty)M_w}{T_\infty^2 R}\right]e^{-\phi} \text{ with } \mathcal{D}_w = \tfrac{1}{2}\mathcal{D}X_\infty\theta^2 e^{-\theta/T_\infty}; \tag{41}$$

it is to be solved under the boundary conditions

$$\phi = Le^{M_w}(-M_1 + M_w/R)T_\infty^2 + \ldots \text{ as } R \to 0, \ \phi = o(1) \text{ as } R \to \infty, \tag{42}$$

the first of which comes from matching with the expansion coefficients (39) for finite r.

Since the problem is well posed under the weaker condition

$$\lim_{R \to 0} R\phi = Le^{M_w}M_w/T_\infty^2, \tag{43}$$

it follows that

$$M_1 = \lim_{R \to 0}(M_w/R - T_\infty^2\phi/Le^{M_w}) \tag{44}$$

can be calculated as a function of $\mathcal{D}_w$, thereby determining the response. The relation between the scaled parameters $(Le^{M_w}/T_\infty^2)M_1$, $(M_w^2 L^2 e^{2M_w}/T_\infty^4)\mathcal{D}_w$ depends only on

$$\beta = (T_a - T_\infty)/Le^{X_v}; \tag{45}$$

figure 4 shows the corresponding response for several positive values of β. It is found numerically, but has never been proved, that the curve does not turn for non-positive values of β, consistent with the conjecture that the inequality (9) must hold for an S-response.

It is worth noting that D is $O(\vartheta^3 e^{\theta/(T_\infty + \gamma X_\infty)})$ at extinction compared to $O(\theta^{-2} e^{\theta/T_\infty})$ at ignition, so that E lies to the left of I, as required. The part between the ignition and extinction points, i.e. the middle branch of the S, will not be discussed here because it is very similar to that for the counterflow diffusion flame (section 8.4.). Again the partial-burning and premixed flames occur, with the same structures for their reaction zones. Since the stability analysis of the branch is confined to the reaction zones, it is the same here as in section 8.5, so no further discussion is necessary.

4. Surface Equilibrium

There are at least two ways in which the fuel can be supplied as a liquid at the surface: the sphere can be completely liquid, i.e. a fuel drop, or it can be a liquid-saturated porous solid. Whatever the method of supply, it is difficult to justify prescription of the surface temperature T_s unless we abandon the specification of L. Maintaining a value of T_s would, in general, require heating or cooling the liquid at the surface, and that would upset the heat balance represented by the boundary condition (10c). Prescription of surface temperature should, more realistically, be replaced by the requirement of liquid-vapor equilibrium at the surface, i.e. the Clausius-Clapeyron relation

$$Y_s = (T_s/T_b)^\beta e^{\hat{\theta}/T_b - \hat{\theta}/T_s} \quad \text{with } \beta, \theta \text{ consts..} \tag{46}$$

Here T_b is the boiling temperature, i.e. the value of T_s for which $Y_s = 1$; it is related to the pressure level in the combustion field by

$$T_b^\beta e^{-\hat{\theta}/T_b} = p_c/k \quad \text{with} \quad k = \text{const..} \tag{47}$$

In order to transform the Clausius-Clapeyron relation into a temperature condition, we eliminate Y_s between it and the Shvab-Zeldovich relation, (7) to obtain

$$2(T_s/T_b)^\beta e^{\hat{\theta}/T_b - \hat{\theta}/T_s} = 2-L+(T_\infty - T_s + L - 2)e^{-M}. \tag{48}$$

This replaces the boundary condition (10b'; clearly T_s changes with M.

Determination of the response $M(\mathcal{D})$ now requires that T_s be calculated afresh for each point. In general, iterations are involved because the structure problem determing M as a function of $\mathcal{D}$ contains T_s (see, for example, the definitions (36)). Different results are obtained according to the way in which $\mathcal{D}$ is varied, via p_c or the radius a of the sphere, the reason being that p_c appears in the boundary condition (48) through T_b. (Since ρ_r has been taken proportional to p_c, and M_r inversely proportional to the radius a of the sphere, the definition (2.23b) shows that $\mathcal{D}$ is proportional to $p_c^\gamma a^2$.)

Normandia and Ludford have considered the response when $\mathcal{D}$ is varied via a. In particular, they find that the curve is again S-shaped when the inequalities (9), (13b) are satisfied by the T_s corresponding to small $\mathcal{D}$, i.e. the solution of equation (48) when M has the value (12b). (There is always such a solution, satisfying the left inequality automatically.) The previous analysis (for T_s fixed) is qualitatively, but not quantitatively, correct: while extinction and ignition analyses can be performed as in section 3, figures 3 and 4 cannot be carried over because the variations in T_s, though only $0(\theta^{-1})$ on the upper and lower branches

of the S-response, modify the extinction and ignition values. These modifications have been worked out by Normandia and Ludford.

The results are strikingly different when D is varied via p_c, as Janssen & Ludford (1983a) have shown. The S is replaced by the rather odd shapes in figure 5, which covers the practical cases of heat being conducted to the environment. These responses were so unexpected that, to obtain more confidence in their validity, numerical integrations of the problem (10a,c,d, 48) were performed for $\vartheta = 10$. In every instance, the numerical results confirmed the essential features of the asymptotic responses. Nothing similar has apparently been obtained in combustion theory, and certainly not in previous studies of diffusion flames.

Two features of these responses deserve to be pointed out, since they contradict conventional wisdom. First, the Burke-Schumann value (17) is not attained on any of the curves as $D \rightarrow \infty$. The Burke-Schumann solution discussed in section 1 is considered a good approximation since in practice D is large. But, instead of standing off from the sphere for high pressures, separating equilibrium regions, the flame sheet actually moves to the surface, forming the second (Buckmaster) equilibrium limit mentioned in connection with the condition (20). Secondly, the burning rate decreases over most of each response, whereas the general belief is that it should increase. Negative slope of the response curve is thought to be inevitably associated with instability, and indeed we found that to be the case for the S-response at the end of section 3. But experience refutes such a conclusion here: by and large, fuel drops do burn steadily.
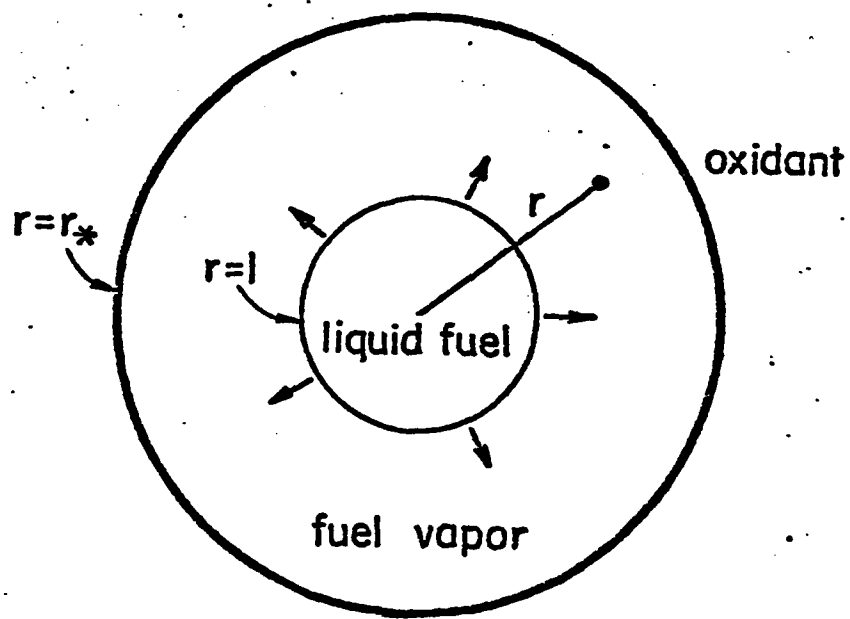
A physically reasonable range of pressures focuses attention on the left ends of the curves in figure 5, and there the decrease of burning rate with pressure is by no means insignificant. Moreover, the computed response curve for methanol over the range .002 to 500 atmospheres clearly shows the steady decline (Janssen & Ludford 1983b). Experiment should therefore be able to give a clear-cut decision on the physical reality of this unexpected phenomenon.
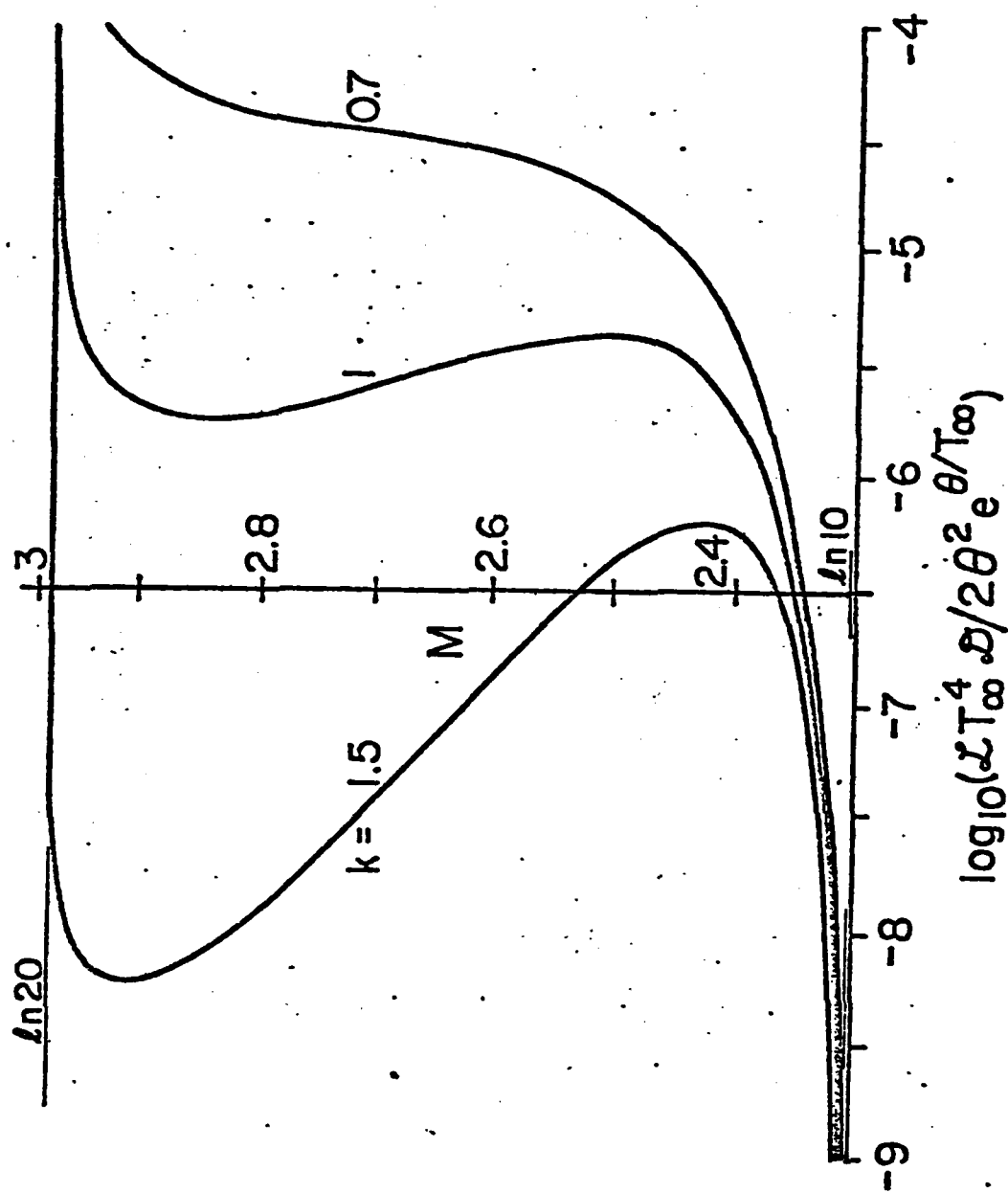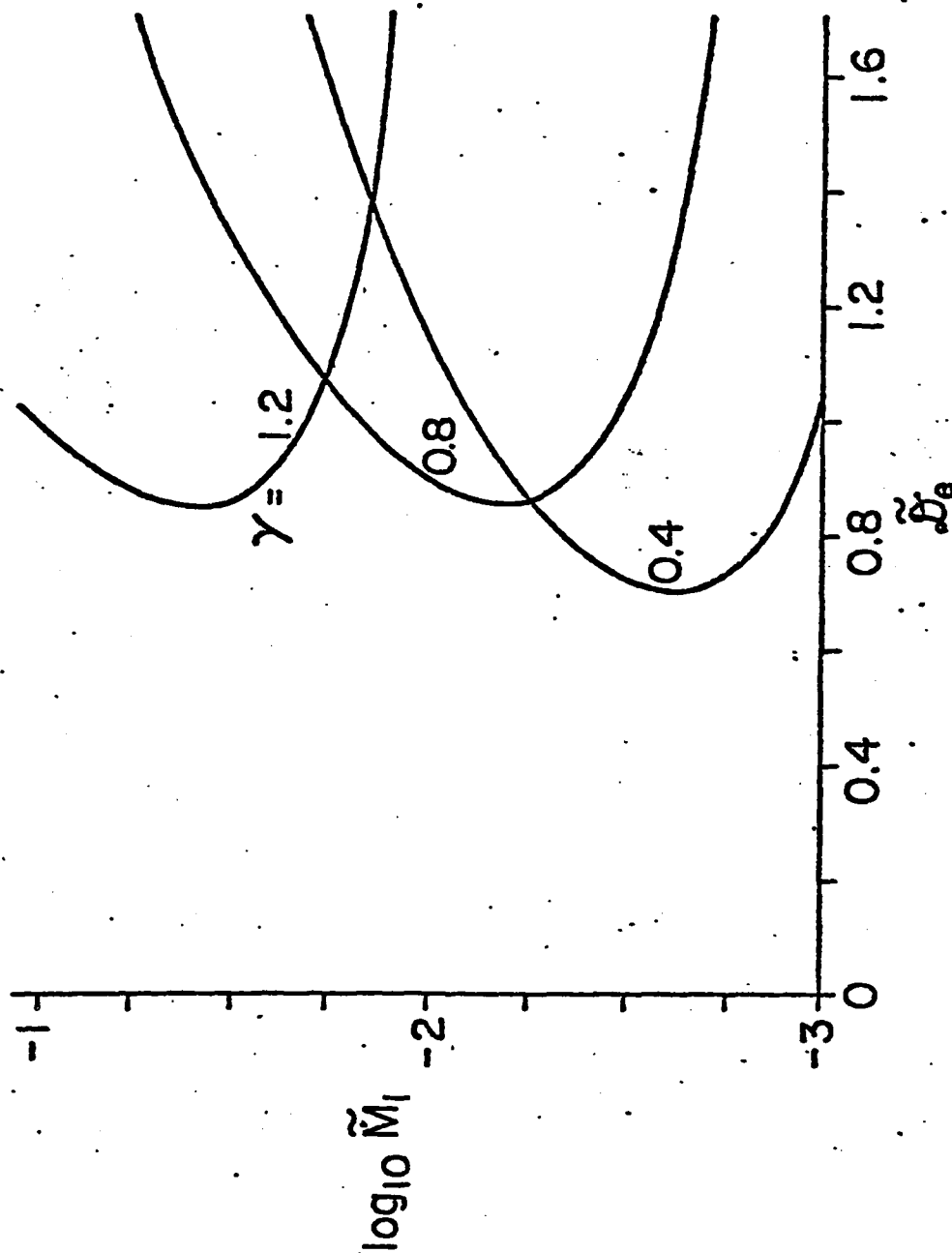
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1. Janssen, R.D. & Ludford, G.S.S. (1983a). The response to
    ambient pressure of fuel drop combustion with surface equili-
    brium. (Submitted for publication.)

2. Janssen, R.D. & Ludford, G.S.S. (1983b). Burning rate
    response of a methanol drop to ambient air pressure. In
    Nineteenth International Symposium on Combustion (in press).
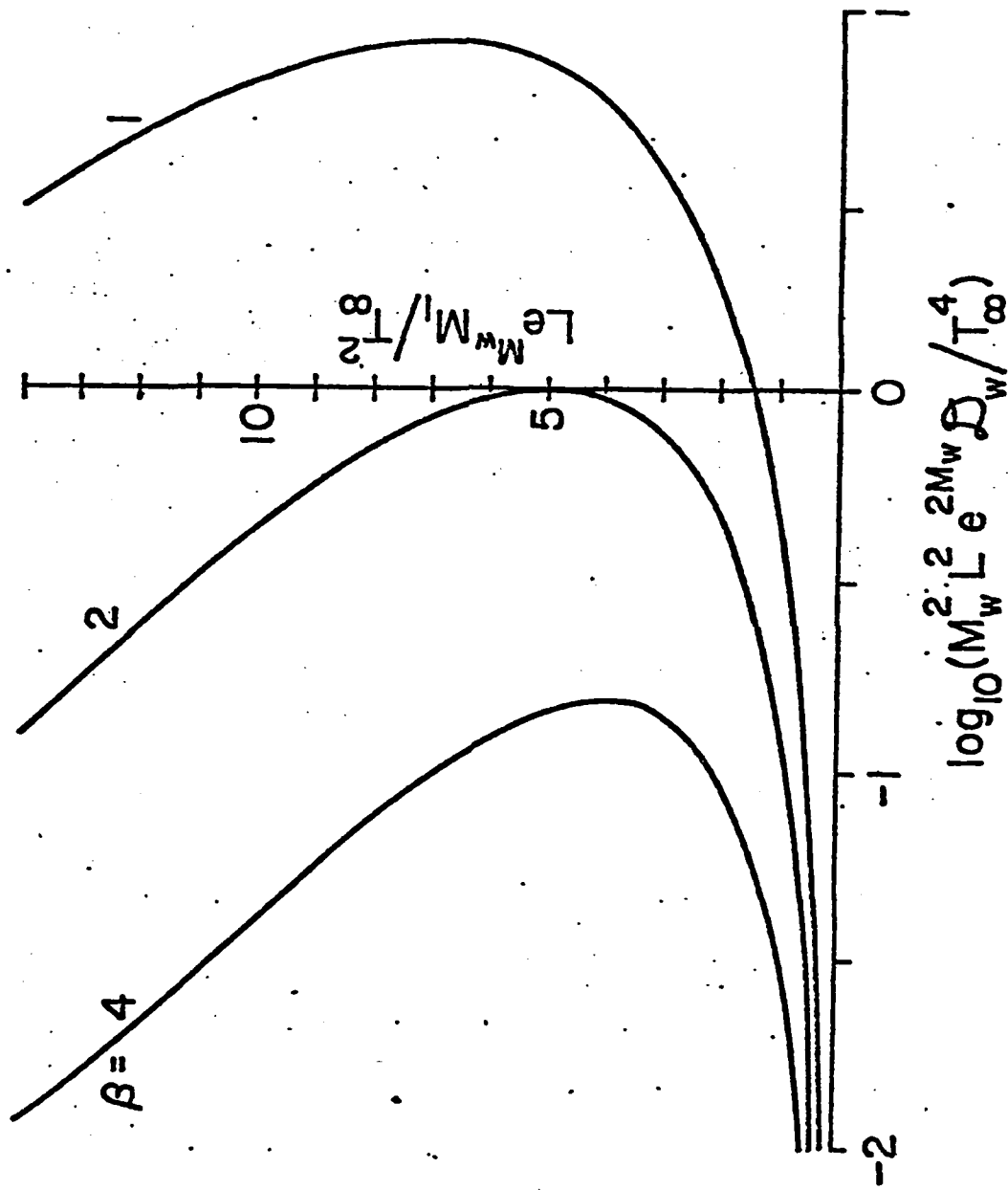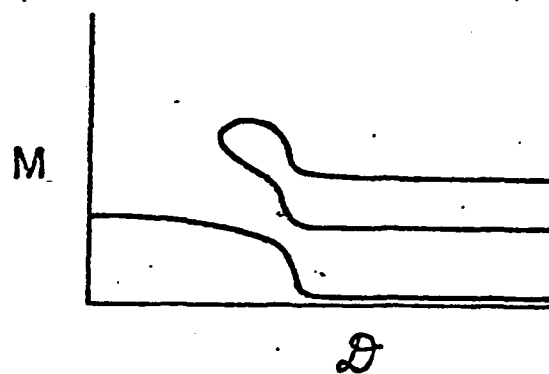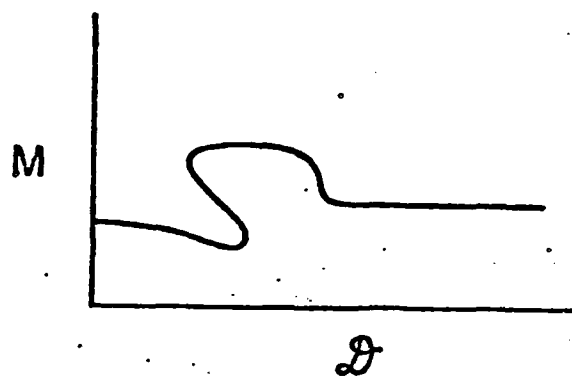   Pittsburgh: The Combustion Institute.

Figure Captions

9.1 Burning fuel drop.

9.2 Steady-state responses when the combustion is nearly adiabatic. Drawn for $L = 0.2$, $T_\infty = 0.2$, $X_\infty = 1$.

9.3 Extinction curves. For $\gamma \leq 0$ no turning point is found numerically.

9.4 Ignition curves. For $\beta \leq 0$ no turning point is found numerically.

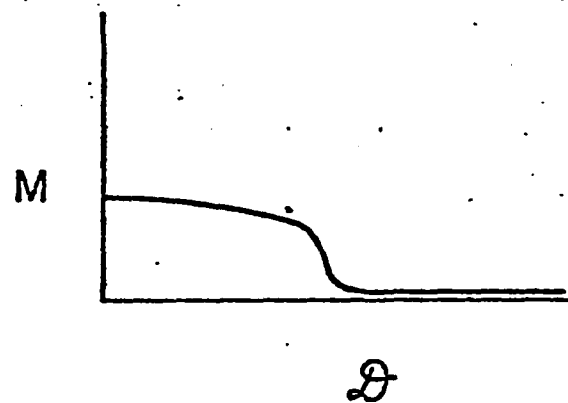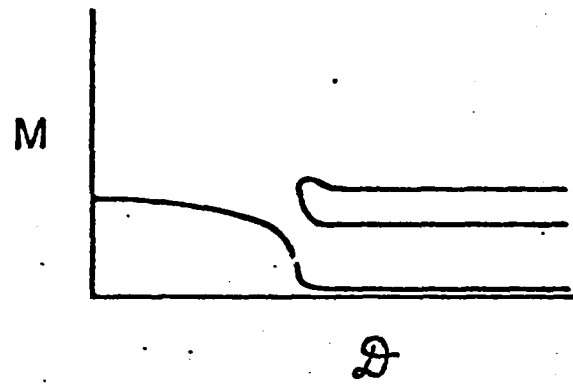9.5 Sketch of steady state responses when there is surface equilibrium.

$\log_{10}(\mathcal{L} T_\infty^4 \mathcal{D}/2\dot\theta^2 e^{\theta/T_\infty})$

M

$\mathcal{D}$

M

$\mathcal{D}$

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Law has shown that the analysis of spherical diffusion flames is quite
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